

# On a Conjecture of Goriely for the Speed of Fronts of the Reaction–Diffusion Equation

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## Abstract

In a recent paper Goriely considers the one-dimensional scalar reaction–diffusion equation  $u_t = u_{xx} + f(u)$  with a polynomial reaction term  $f(u)$  and conjectures the existence of a relation between a global resonance of the hamiltonian system  $u_{xx} + f(u) = 0$  and the asymptotic speed of propagation of fronts of the reaction diffusion equation. Based on this conjecture an explicit expression for the speed of the front is given. We give a counterexample to this conjecture and conclude that additional restrictions should be placed on the reaction terms for which it may hold.

82.40.Ck, 47.10+g, 3.40Kf, 2.30.Hq

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## I. INTRODUCTION

The one dimensional scalar reaction-diffusion equation

$$u_t = u_{xx} + f(u) \tag{1}$$

with  $f(0) = f(u_+) = 0$  has been the subject of much study not only because it models different phenomena [1–3], but also because it is the simplest reaction-diffusion equation for which rigorous results can be obtained [3,4,6,5,7–11]. Depending on the situation being considered the reaction term  $f(u)$  satisfies additional properties. It has been shown for different classes of reaction terms that suitable initial conditions  $u(x, 0)$  evolve in time into a monotonic front joining the state  $u = u_+$  to  $u = 0$ . The asymptotic speed at which the front travels is the minimal speed for which a traveling monotonic front  $u(z) = u(x - ct)$  exists [5,7]. Traveling fronts are a solution of the ordinary differential equation  $u_{zz} + cu_z + f(u) = 0$ . In the present case we shall be concerned with two types of reaction terms, the classical case  $f > 0$  in  $(0, u_+)$  with  $f'(0) > 0$  and the bistable case  $f < 0$  in  $(0, a)$ ,  $f > 0$  in  $(a, u_+)$  with  $\int_0^{u_+} f > 0$  and  $f'(0) < 0$ . In the classical case there is a continuum of speeds  $c \geq c^*$  for which monotonic fronts exist. The system evolves into the front of speed  $c^*$ . In the bistable case there is a unique isolated value of the speed  $c^*$  for which a monotonic front exists, the system evolves into this front. The problem is to determine the speed of propagation of the front. In the classical case, if in addition  $f'(0) > f(u)/u$  the speed of propagation  $c^*$  is the so called linear or KPP value  $c_{KPP} = 2\sqrt{f'(0)}$  [4]. In the other cases (as well as in the bistable case) there exist variational principles both local and integral from which the speed can be calculated with any desired accuracy for arbitrary  $f$  [3,6,10,11].

In a recent paper [12] Goriely proposes a new method for the determination of the speed. Based on an observed property of some exactly solvable cases, namely reaction terms of the form  $f(u) = \mu u + \nu u^n - u^{2n-1}$  he conjectures that for polynomial reaction terms of the form

$$f(u) = \mu u + g(u) \tag{2}$$

where  $g(0) = g'(0) = 0$  and the polynomial  $g$  independent of  $\mu$ , the speed of the front can be calculated from the knowledge of the heteroclinic orbit of the Hamiltonian system

$$u_{zz} + f(u) = 0.$$

This property of solvable cases had not been observed before. The purpose of this article is to show by means of a counterexample that this conjecture is not true in general for the above class of polynomial reaction terms. However, considering that the conjecture is indeed true for a large class of reaction terms (the solvable cases mentioned above), it is a very interesting unsolved problem to characterize the class of functions for which it is valid. For the sake of clarity we state the conjecture here. The conjecture makes use of the fact the front approaches the equilibrium state  $u = 0$  as  $e^{\lambda_- z}$ , a well established fact, and approaches the equilibrium point  $u = u_+$  as  $u = u_+ - Le^{\gamma_+ z}$ , an assumption which is not always satisfied. Then the global resonance, defined as

$$\delta = -\frac{\gamma_+}{\lambda_-} \tag{3}$$

is conjectured to be a constant, for a general class of polynomial reaction terms, at all values of  $\mu$  for which the nonlinear front exists. Explicit expressions are known for the rates of approach  $\gamma_+$  and  $\lambda_-$  in terms of  $c$  and  $f$  therefore, if  $\delta$  can be calculated at any point, then an analytic formula for the speed can be obtained. There is such a point where it can be calculated, and that is the point at which  $c = 0$  and the system is hamiltonian. There is a unique value  $\mu < 0$  for which such a front exists, (we shall label it as  $\mu_h$  and the corresponding equilibrium point as  $u_h$ ) and therefore the speed is completely determined. In the following section we consider a specific polynomial reaction term and show that it fails to satisfy the conjecture.

## II. THE COUNTEREXAMPLE

Consider the reaction term  $f(u) = \mu u + 2u^2 - 7u^3 + \frac{20}{3}u^4 - 2u^5$ . This is of the form  $f(u) = \mu u + g(u)$  where the polynomial  $g(u) = 2u^2 - 7u^3 + 20u^4/3 - 2u^5$  satisfies the

properties  $g(0) = g'(0) = 0$  and is independent of  $\mu$  as requested by the conjecture. For the hamiltonian system

$$u_{zz} + \mu u + 2u^2 - 7u^3 + \frac{20}{3}u^4 - 2u^5 = 0$$

a heteroclinic orbit joining two equilibrium points exists at the value  $\mu = \mu_h = -0.153897$ . In Fig. 1 the reaction term  $f(u)$  is shown together with the (scaled) potential. It is clear that a heteroclinic solution joining the point  $u = 0$  to  $u_+ = u_h = 0.262156$  exists. In this case the resonance  $\delta$  can be calculated. Its value is given by

$$\delta = \delta_h = \sqrt{\frac{f'(u_h)}{\mu_h}} = 0.865558. \quad (4)$$

Let us now consider the propagating fronts which are a solution of

$$u_{zz} + cu_z + \mu u + 2u^2 - 7u^3 + \frac{20}{3}u^4 - 2u^5 = 0.$$

Before giving the results of the numerical and analytical calculations we show the plot of the function  $f$  at several values of  $\mu$  which will make clear the numerical and analytical results that follow. As  $\mu$  increases the equilibrium point  $u_+$  increases until at  $\mu = 1/3$  it reaches the value  $u_+ = 1$  where  $f' = 0$ . Above this value of  $\mu$  there is a discontinuous jump in  $u_+$ , the front joins the origin  $u = 0$  to a new fixed point which corresponds to a different root of the polynomial  $f(u)$ . In Fig. 2 we show the function  $f$  at different values of  $\mu$ . At  $\mu = 1/3$  the fixed point  $u_+ = 1$  and the derivative  $f'(u_+) = 0$ . At  $\mu = 0.4$ , we see that the value of  $u_+$  is now the new root of  $f$  which did not exist at low values of  $\mu$ .

First we describe the results of the numerical integrations of the initial value problem for Eq(1) with sufficiently localized initial value perturbations  $u(x, 0)$ . The speed is obtained numerically and the value of  $\delta$  is then computed from Eq.(3) which can be expressed as [12]

$$\delta = \frac{-c + \sqrt{c^2 - 4f'(u_+)}}{c + \sqrt{c^2 - 4f'(0)}}. \quad (5)$$

In Fig. 3 we show the asymptotic speed of the front as a function of  $\mu$ . The solid line gives the numerical results and the dashed line corresponds to the linear or KPP value  $2\sqrt{\mu}$ . First we observe that the KPP value is lower than the calculated speed in the range of  $\mu$  shown

which means that the transition to the linear or KPP regime occurs at larger values of  $\mu$ . Even though the value of  $u_+$  is discontinuous, the speed is a continuous function of  $\mu$ .

And finally the graph of the resonance  $\delta$  as a function of  $\mu$  is shown in Fig. 4. At  $\mu = \mu_h$  it adopts the analytically calculated value from the hamiltonian case, decreases to a value  $\delta = 0$  at  $\mu = 1/3$  jumps discontinuously to a larger value and increases from there on. This discontinuity can be attributed to the discontinuity in  $u_+$ . At the value of  $\mu = 1/3$  where  $f'(u_+) = 0$  it is evident from Eq (5) that  $\delta = 0$ . As we will show below, at this value of  $\mu$  the speed and the asymptotic behavior for the front can be calculated analytically and it is found that the front does not approach the fixed point  $u_+ = 1$  exponentially, therefore one of the assumptions of the conjecture does not hold. Indeed we shall show that at  $\mu = 1/3$  the front approaches  $u = 1$  as  $u \sim 1 - A/z$ .

In order to determine the speed we shall make use of variational principles. It is known that the speed of the front is given by [10]

$$c = \max 2 \frac{\int_0^{u_+} \sqrt{-f\phi\phi'} du}{\int_0^{u_+} \phi du} \quad (6)$$

where the maximum is taken over positive decreasing functions  $\phi(u)$ . Taking as a trial function

$$\phi(u) = \frac{(1-u)^{7/2}}{\sqrt{u}} e^{-3/[(2(1-u))]}$$

the integrals in Eq.(6) can be performed. We obtain for  $\mu = 1/3$

$$c \geq \sqrt{\frac{3}{2}} > 2\sqrt{\mu}.$$

To obtain an upper bound we make use of the local variational principle [6]

$$c = \inf_{\rho} \sup_u \left( \rho'(u) + \frac{f(u)}{\rho(u)} \right)$$

where the trial function  $\rho(u) > 0$  and  $\rho'(0) > 0$ . Choosing as a trial function  $\rho(u) = \sqrt{2/3} u (1-u)^2$  we obtain the upper bound

$$c \leq \sqrt{\frac{3}{2}}$$

which combined with the above lower bound implies that the speed is exactly  $c = \sqrt{3/2}$  in agreement with the results of the numerical integration. The exact value of the speed could be obtained analytically from the variational principles due to the fact that for  $\mu = 1/3$  the derivative of the front can be calculated exactly. The derivative of the front as a function of  $u$ ,  $p(u) = -du/dz$  satisfies the equation  $p(u)p'(u) - cp(u) + f(u) = 0$  and the exact solution at  $\mu = 1/3$  is given by  $p(u) = \sqrt{2/3} u (1 - u)^2$ . With this expression for  $p$  we may calculate the approach to the fixed point  $u = 1$ . Near  $u = 1$ ,  $p \sim \sqrt{2/3} (1 - u)^2$  so that

$$\frac{du}{dz} \sim -\sqrt{\frac{2}{3}} (1 - u)^2$$

from where it follows that

$$u(z) \sim 1 - \sqrt{\frac{3}{2}} \frac{1}{z}.$$

We see then that at this point  $\delta = 0$  since the rate of approach is not exponential but algebraic and one of the assumptions of the conjecture is not satisfied. We conclude from this example that the conjecture does not hold for general polynomials of the form given by Eq.(2).

### III. CONCLUSION

We have seen by means of a counterexample that the conjecture put forward that relates certain properties of the hamiltonian system  $u_{zz} + f(u) = 0$  with the speed of the front solution of  $u_{zz} + cu_z + f(u) = 0$  is not satisfied by general polynomial reaction terms  $f(u)$ . As observed by Goriely, there is a class of reaction terms for which it does hold, those for which an exact solution for the front  $u(z)$  can be given explicitly. Numerical evidence has been given [12] in at least one case where the conjecture seems to hold in a case where the front cannot be calculated explicitly. On the other hand, we have given a counterexample to this conjecture. It is an interesting problem to establish precisely the conditions under which the proposed conjecture holds. This would lead to a classification of systems in at least three classes, those for which the speed is given in terms of the derivative at one fixed

point, that is the KPP value  $c = 2\sqrt{f'(0)}$ , those in which the speed would be determined by the derivatives at the two fixed points (the expression given by Goriely would hold) and the rest, for which the speed depends on integral properties of the reaction term.

#### IV. ACKNOWLEDGMENTS

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## Figure Captions

### Figure 1

Graph of the reaction term  $f$  and the corresponding scaled potential at the value of  $\mu$  for which the speed of the front vanishes and the system is hamiltonian.

### Figure 2

Graph of the reaction term at different values of  $\mu$ . The value of the stable point increases with  $\mu$  until  $\mu$  reaches  $1/3$ . A discontinuous jump in the stable point occurs at that value.

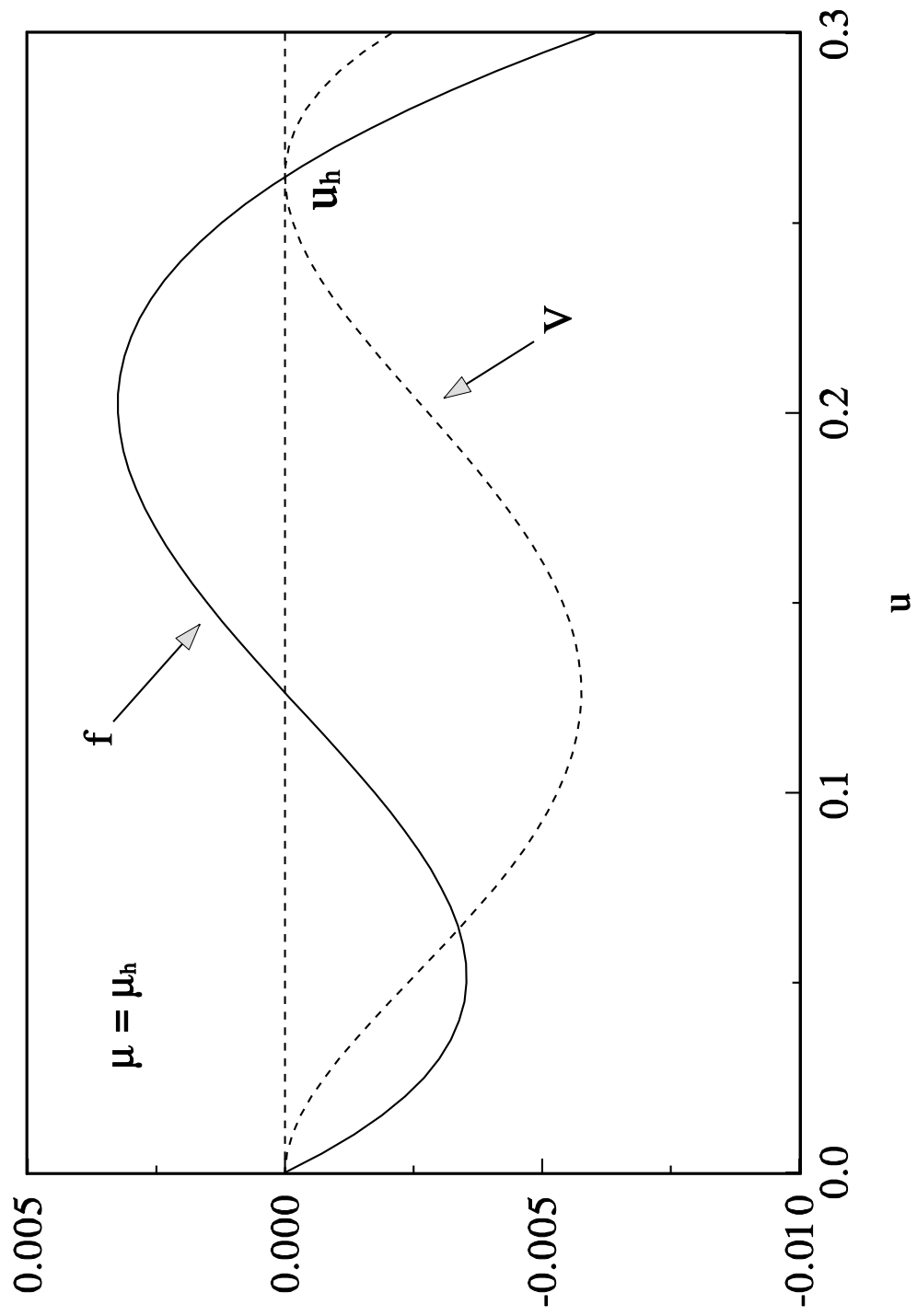
### Figure 3

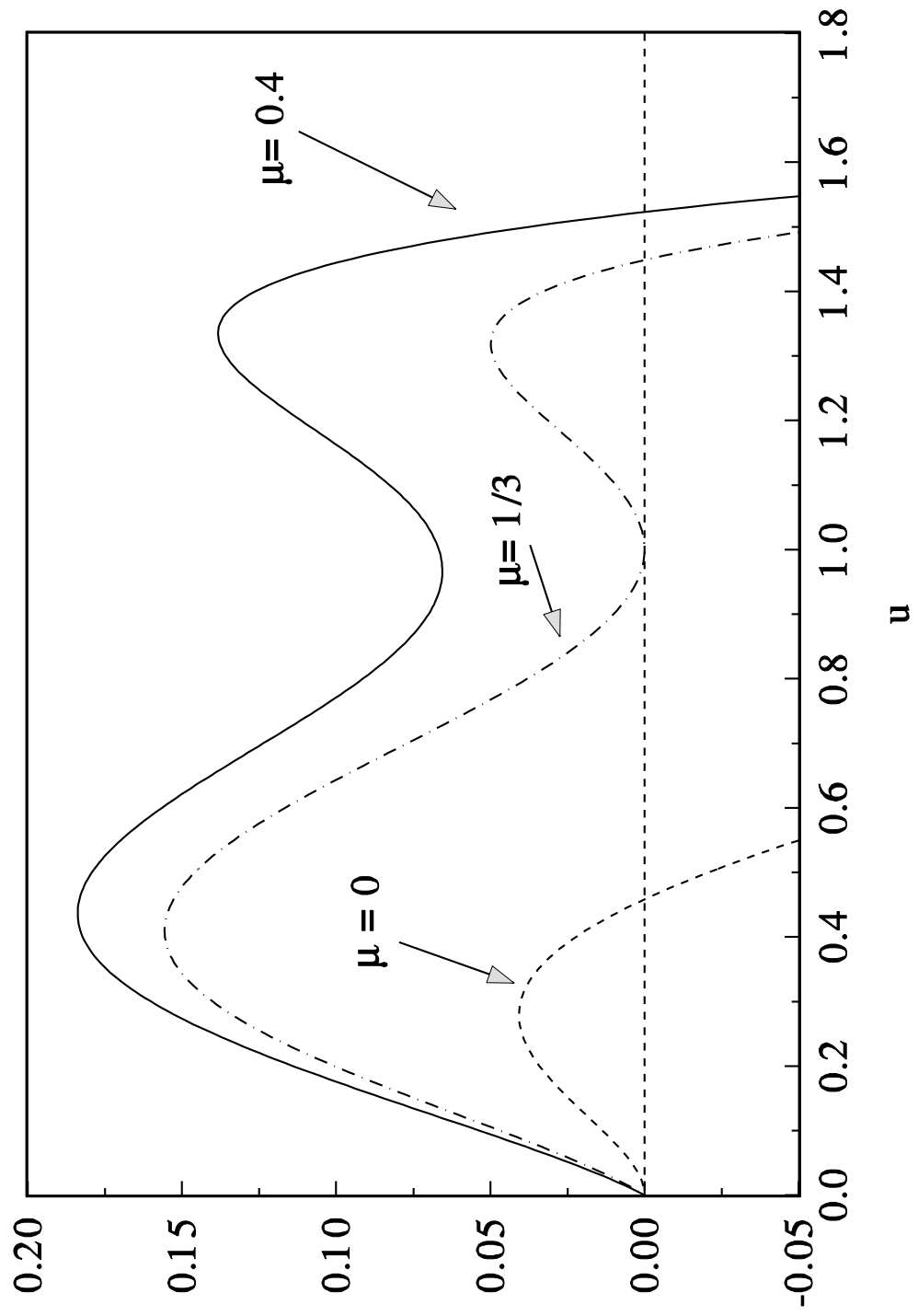
Graph of the speed obtained from the numerical integration of the initial value problem. The speed of the front is a continuous function of  $\mu$ . In the range of  $\mu$  shown the speed is greater than the linear or KPP value.

### Figure 4

Value of the resonance  $\delta$  as a function of  $\mu$  obtained from the numerical integrations.

Figure 1





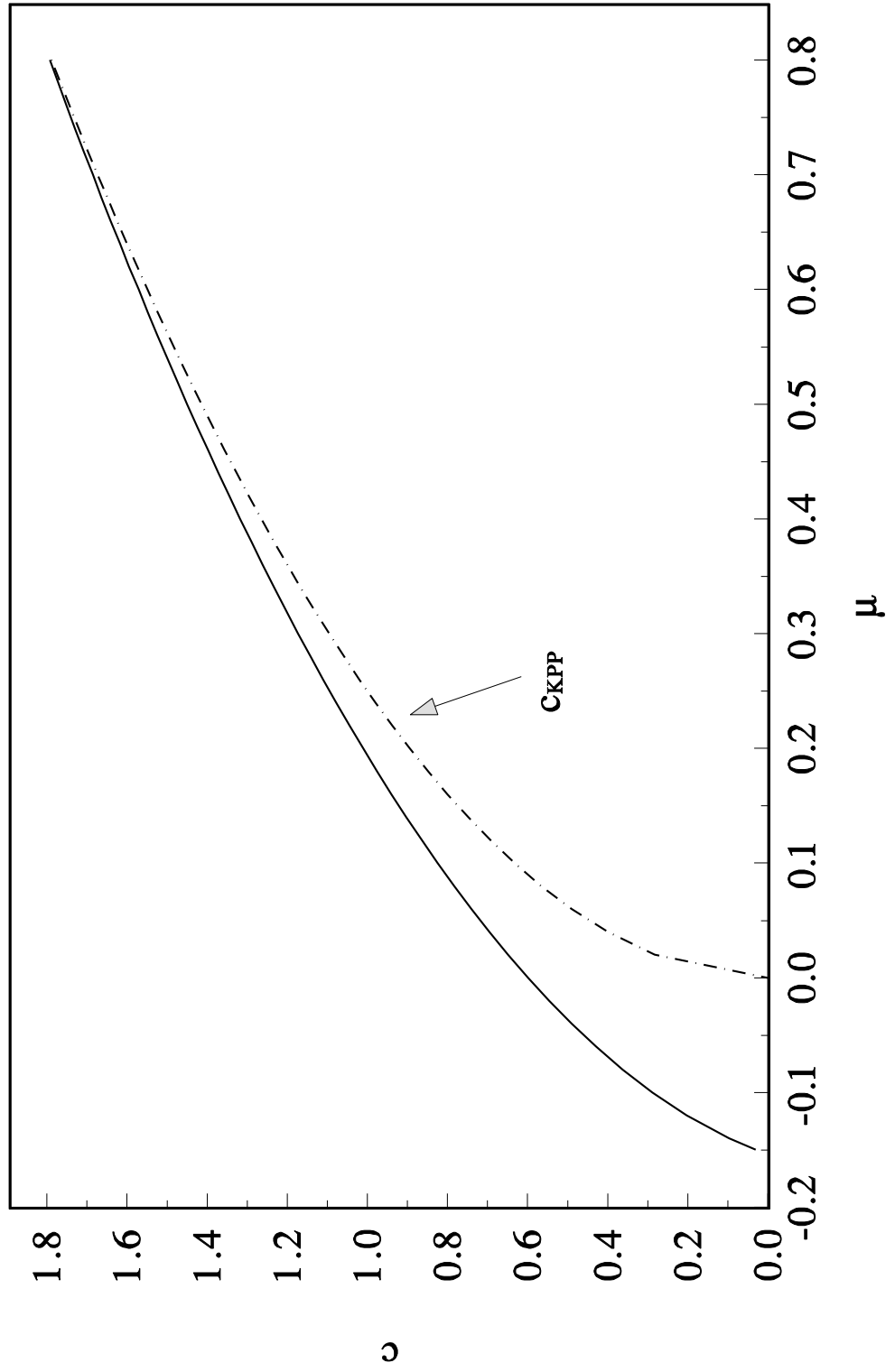


Figure 4

